Scientific Computer Programming for Evaluation of Nuclear Data

D. MacMahon†, E. Schönfeld‡, S.Y.F. Chu, and E. Browne

The Isotopes Project, a member of the international Decay Data Evaluation Project (DDEP) [1], has significantly contributed to the methodology and development of computer programs for data analysis.

The evaluation of data that are statistically discrepant ($\chi 2/\nu >> 1$) is a usual problem for evaluators. Several methods have been developed [2] during the years to produce a recommended *average* from a set of discrepant data. The DDEP has adopted the *Limitation of Relative Statistical Weights* [3] method, and the Isotopes Project, in collaboration with the Centre for Analytical Research in the Environment (CARE), Imperial College, London, UK, developed LWEIGHT, a computer program to perform the calculations. This program, which identifies statistical outliers, calculates *recommended averages* and their *uncertainties* for several sets of input data. LWEIGHT, written in Fortran 77 for PC's, runs in DOS only, and is available on diskette.

The electron-capture decay process produces vast amounts of X-rays from atomic-shell vacancies that are subsequently filled by electrons from outer shells. The emission probabilities of these X-rays are often *calculated* rather than *measured*. For such calculation, however, one needs to know the relative electron-capture probabilities to the individual atomic subshells. Schönfeld [4] derived the formulas to calculate these quantities for allowed and first-forbidden non-unique transitions. Again, the Isotopes Project in collaboration with the Physicalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany, developed EC-CAPTURE, and interactive computer program that uses Schönfeld's formalism to calculate relative electron-capture probabilities to individual subshells. The program, written in Fortran 90 for PC's, runs in Windows95 and NT only, and is available on diskette.

Footnotes and References

† Centre for Analytical Research in the Environment (CARE), Imperial College, London, UK.

‡ Physicalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany.

1. E. Browne and the Decay Data Collaboration, *International Decay Data Evaluation Project*, Nuclear Science Division 1997 Annual Report.
2. M.U. Rajput and T.D. MacMahon, *Techniques for evaluating discrepant data*, Nucl. Instr. and Meth. in Phys. Res. **A312**, 289 (1992).
3. M.J. Woods and S. Munster, National Physical Laboratory, Teddington, UK, Report No. RS(EXT)95, 1988.
4. E. Schönfeld, Tables for the Calculation of Electron Capture Probabilities, Report PTB-Laborbericht 6.33-95-22, 1995.